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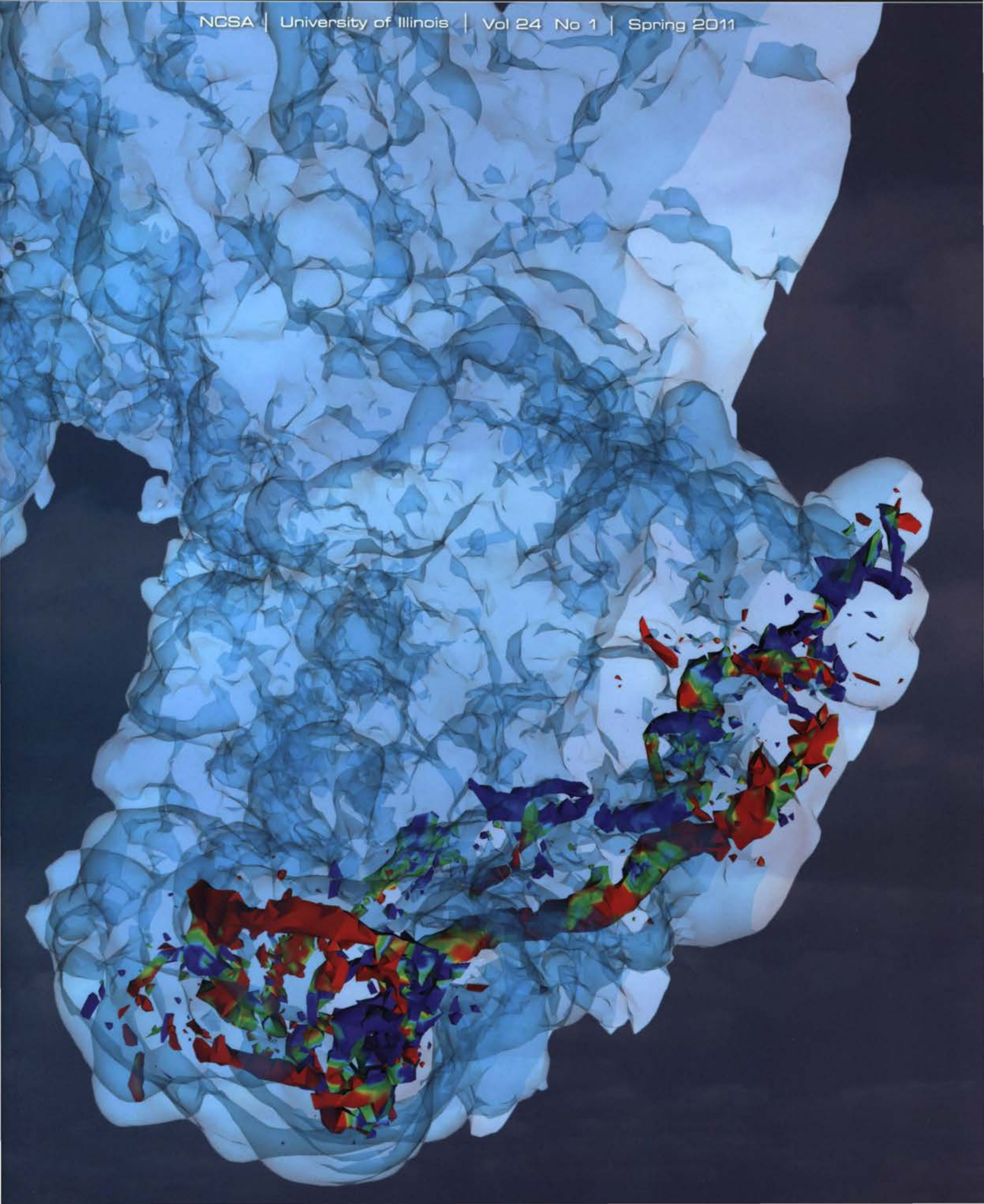

NCSA

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Who we are

The University of Illinois at Urbana-Champaign's National Center for Supercomputing Applications (NCSA), one of the five original centers in the National Science Foundation's Supercomputer Centers Program, opened its doors in January 1986. Over the years NCSA has contributed significantly to the birth and growth of the worldwide cyberinfrastructure for science and engineering, operating some of the world's most powerful supercomputers and developing the software infrastructure needed to efficiently use them.

That tradition continues as the center, Illinois, IBM, and their partners in the Great Lakes Consortium for Petascale Computation develop what is expected to be the first computer dedicated to open scientific research capable of sustaining more than one petaflop, or one quadrillion calculations per second. Called Blue Waters, the system will be dedicated to massive simulations and data analysis projects that will improve our society, health, environment, and economic competitiveness. NCSA and the consortium will also work with research communities to create the new software technologies, scientific applications, and educational programs needed to take full advantage of this new system.

Blue Waters will benefit from NCSA's ongoing focus on cyberenvironments, cyber-resources, and innovative systems research. Cyberenvironments give research communities the means to fully exploit the extraordinary resources available on the internet (computing systems, data sources and stores, and tools). Cyber-resources ensure computing, data, and networking resources are available to solve the most demanding science and engineering problems and that the solutions are obtained in a timely manner. Innovative systems research involves testing and evaluating the performance of emerging computing systems for scientific and engineering applications.

The center also leaves its mark through the development of networking, visualization, storage, data management, data mining, and collaboration software. The prime example of this influence is NCSA Mosaic, which was the first graphical Web browser widely available to the general public. NCSA visualizations, meanwhile, have been a part of productions by the likes of PBS's NOVA and the Discovery Channel. Through its Private Sector Program, top researchers explore the newest hardware and software, virtual prototyping, visualization, networking, and data mining to help U.S. industries maintain a competitive edge in the global economy.

Support for NCSA is provided by the National Science Foundation, the state of Illinois, industrial partners, and other federal agencies. For more information, see **www.ncsa.illinois.edu**.

On the cover

Commercial aircraft can affect climate by changing cloud cover through the production of contrails. Using large eddy simulations, Stanford University researchers are building better models of the contrail formation process to help understand the effect of these human-made clouds on climate. These visualizations of simulation results show the evolution of the aircraft wake vortices (opaque surfaces) and how they spread the jet exhaust material (transparent surfaces) that forms the contrail. The complex dynamics of the vortices must be simulated accurately to predict how the contrail will spread across the sky. *See the Parting Shot on page 28 to learn more.*

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02 The "Most Powerful Supercomputer in the World"
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Director, NCSA

An Expert Opinion

THE "MOST POWERFUL COMP

LAST FALL OUR CHINESE SUPERCOMPUTING COLLEAGUES caused a stir in the United States, as well as the rest of the world, by announcing the Tianhe-1A supercomputer. Tianhe-1A, with a Linpack benchmark score of 2.57 petaflop/s (PF/s), captured the #1 spot on the Top500 List, shoving aside Oak Ridge's Jaguar at 1.76 PF/s. Tianhe-1A was even referred to in President Obama's State of the Union address on January 25: "just recently, China became the home to ... the world's fastest computer." The rapid rise of China in the Top500 rankings (another Chinese supercomputer (Nebulae) is #3 in the Top500 list) is indicative of the significant investments of China in high-performance computing—investments that encompass education and research in a broad range of HPC technologies. There is no doubt that China is catching up fast, but one should not relegate the United States to a second-class spot in supercomputing so quickly.

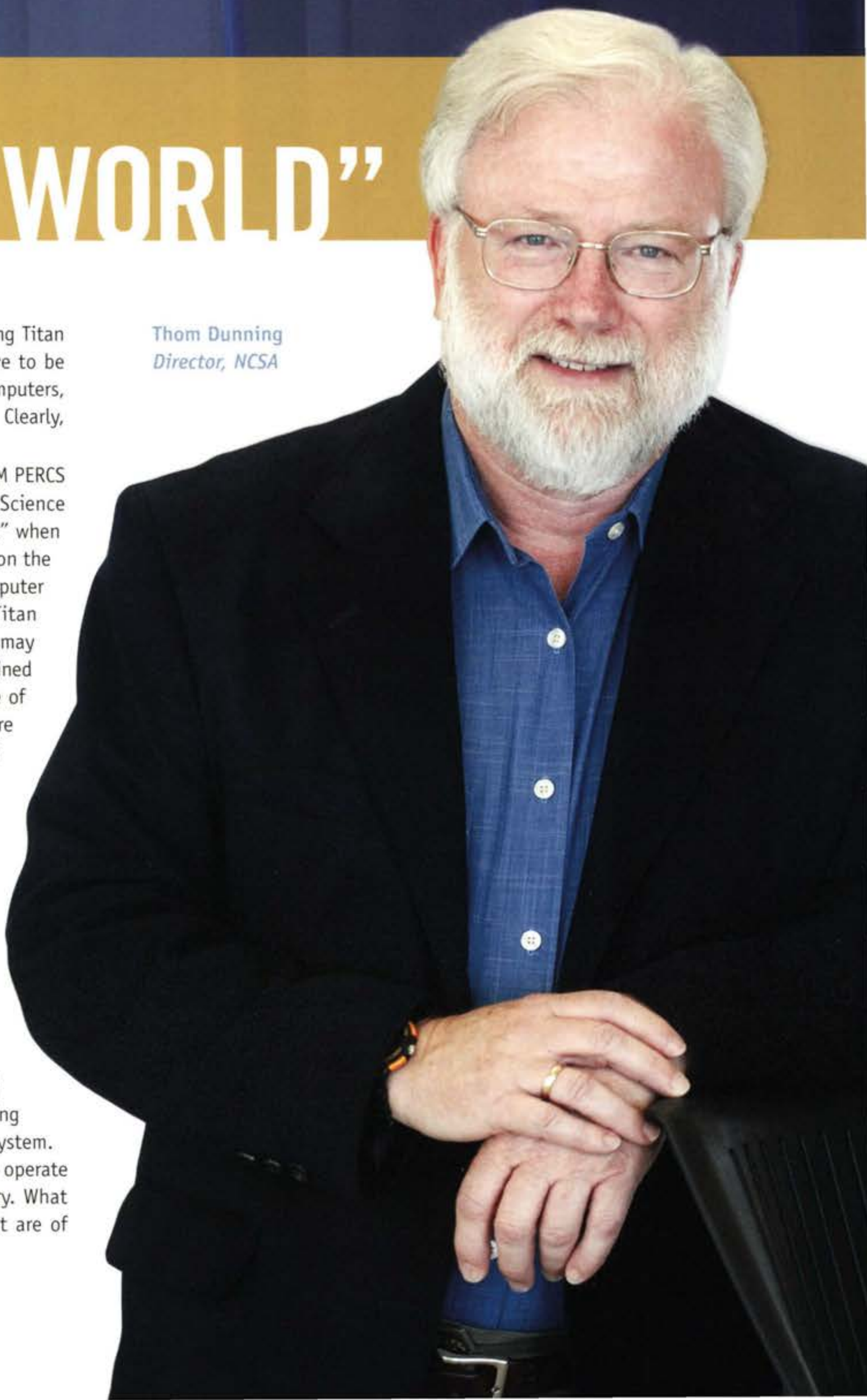
Tianhe-1A achieves a peak performance of 4.70 PF/s by deploying 7,168 NVIDIA Fermi GPUs in addition to 14,336 Intel Nehalem CPUs. Nearly 80 percent of Tianhe-1A's performance comes from the GPUs. The problem is—at the present time—there are few science and engineering applications that can take full advantage of the massive numerical performance of GPUs. So, the performance of Tianhe-1A on nearly all existing science and engineering applications will only be a fraction of that achieved on the Linpack benchmark. As a result Jaguar, despite its #2 ranking on the Top500 List, will likely outperform Tianhe-1A by a substantial margin on most current science and engineering applications. The extraordinary performance provided by GPUs is certainly of interest in our country. In fact, NCSA will shortly be deploying its second NSF-allocated CPU-GPU system to enable further exploration and use of this technology, which is only one part of our HPC ecosystem.

China's achievement highlights a flaw in the metric used to rank supercomputers on the Top500 List. We have long known that the Linpack benchmark was not an ideal metric. It measures just one element of the performance of the computer—its ability to solve a dense system of linear equations. This metric is important in some, but certainly not all, science and engineering applications. Despite attempts by Jack Dongarra, the developer of the Linpack benchmark, and his colleagues to convince the high-performance computing community to use a more comprehensive set of metrics (e.g., the HPC Challenge benchmarks), the community has clung to the Linpack benchmark. This benchmark is, after all, simple and, unlike the HPC Challenge benchmarks, gives a single number, making it straightforward to identify the "most powerful computer." But what does it mean when a computer runs the Linpack benchmark well, but many science and engineering applications poorly?

What is the means of identifying the "most powerful computer" in the world? Unfortunately, it is not simple and the fact that the HPC Challenge benchmarks are underutilized today is an illustration of this difficulty. In addition to high-performance processors, science and engineering applications require a low-latency, high-bandwidth memory subsystem (many scientific applications are memory-bound, not compute-bound) and a low-latency, high-bandwidth processor interconnect (critical for scaling applications to large processor counts). In addition, many science and engineering applications involve substantial movement of data between memory and the file system. So, the performance of the I/O subsystem is also important. The HPC Challenge benchmarks cover most, but not all, of these (and other) critical performance characteristics. But how does one convert a large number of benchmarks, like the HPC Challenge benchmarks, into a composite score to enable the computers to be ranked?

Perhaps the best way to rank the performance of a computer system would be to have it execute an average workload found at a number of supercomputing centers and select the top performing computer using this metric. This is what is done at Lawrence Berkeley's NERSC with their ESP (Effective System Performance) metric, which is regularly used in their computer procurement process. Although this approach works well when comparing computers with similar architectures, it is not easy to apply if there are significant differences in the architectures. In this case, substantial software porting and optimization efforts, similar to those underway at NCSA in support of the Blue Waters petascale computer

UTER IN THE WORLD"

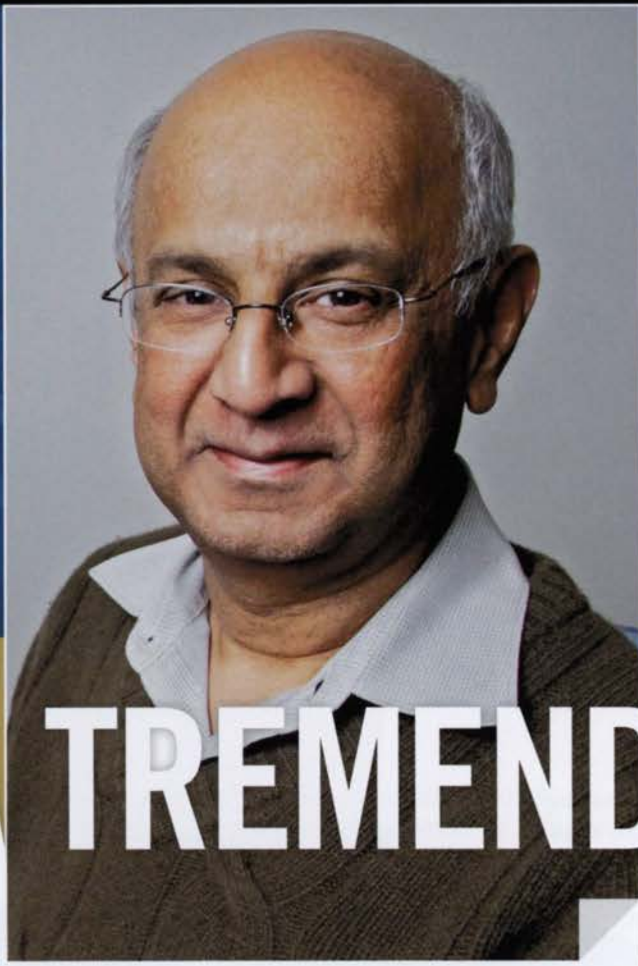


Thom Dunning
Director, NCSA

and at Oak Ridge National Laboratory in support of its upcoming Titan petascale computer (a hybrid CPU-GPU computer), would have to be undertaken to ensure that applications, designed for earlier computers, are taking advantage of the special features of the computer. Clearly, this approach could entail an enormous amount of work.

I will go out on a limb and state that Blue Waters, the IBM PERCS system being deployed by NCSA this year for the National Science Foundation, will be "the most powerful computer in the world" when it officially comes online next year. Will it be the #1 computer on the Top500 List? It may or may not be; the Japanese Kei supercomputer as well as Lawrence Livermore's Sequoia and Oak Ridge's Titan supercomputers and any new computers deployed by China may score higher on the Linpack benchmark. But, with its high sustained (≥1 PF/s) and peak performance (≥10 PF/s) for a broad range of science and engineering applications using powerful eight-core chips (~250 GF/s), high-performance memory subsystem (~5 PB/s) and interconnect (~500 TB/s bisection bandwidth), coupled with its world-class I/O subsystem (≥4 TB/s), Blue Waters will solve a wider range of science problems in less time than any other computer that will be available in the 2012 time frame. Isn't this what we mean when we crown a computer "the most powerful computer in the world?"

So, how can we unambiguously identify the #1 computer in the world? I don't have an answer, but we certainly can't continue to use the one-dimensional Linpack benchmark. The days when this was a useful metric are over. In fact, perhaps we need to ask if a simple type of ranking such as this is relevant today given the wide variety of computational science and engineering problems that are being tackled, each with its own special demands on the computer system. We all want to be ranked at the top spot, but our mission is to operate systems that truly support science and engineering discovery. What is really important is the time to solution for problems that are of importance to you.



A TREMENDOUS RETURN

An expert in building reliable computing systems, Ravi Iyer is the University of Illinois at Urbana-Champaign's vice chancellor for research. NCSA's J. William Bell talked to Iyer recently about the Blue Waters sustained-petascale supercomputer and the role of large projects like Blue Waters and interdisciplinary centers like NCSA at the University.

Q. Tell us a little bit about the role that large-scale projects like Blue Waters that span campus play at a place like Illinois.

A. Let me tell you what was exciting about the Blue Waters project. We had those in scientific computing at NCSA, the major applications researchers, the people who really understood heavy iron computing on the ground. And we could not just go and say, "We'll only do our piece and not do anything else." We really had to work together to build the proposal so that, jointly with IBM, it really was a coherent argument that this system, the Blue Waters machine, would in fact be the best machine possible.

Given that this was a very diverse group, we could make the case that the benefits that would accrue to the country would be much greater putting it in a place that was a computer science and computer engineering powerhouse, as opposed to going and putting it in a national lab or somewhere else where the machine would just be substantially unavailable to others.

I think what was unique is our ability to span this and be able to bring out something transformational to computer science and engineering in this country. That would not have happened without such an eclectic group and this broad array of application experts who worked very closely with the system designers and with IBM.

Q. Applications scientists seem to have high hopes as well.

A. Very high hopes indeed. Throughout the campus and in my travels across the country and internationally, I think, the hope that the world has for Blue Waters is that we'll be able to address these big societal problems and that they will be partners in working with us.

In the end, once the machine is in place, the big story is the major issues—energy, the climate, genetic issues that we have—I mean how can we solve these issues? You need a computing system of this size to start to make a dent in this.

Q. With your vice chancellor for research hat on, what role does that play in Illinois' overall mandate? Facilitating the solution of those societal problems?

A. These kinds of environments, these kinds of centers that address those issues are critical if we are to maintain the competitiveness of the U.S. economy. Without these kinds of investments, we will fall back.

Our friends at IBM call it "building the smarter planet." That needs a level of compute power and a level of smarts in building these machines that doesn't exist today. But it is also engaging our bright young students in that process that [is important].

Q. Is there a synergy there to putting a resource like Blue Waters at a university? Between innovation and education?

A. Students today, and rightly so, are really very keen that their education address some serious and important societal problems—food, energy, water. I can see courses, research projects, proposals going out that now put forward the existence or the availability of a Blue Waters-type of machine as being a resource in addressing these problems.

I see a huge opportunity to engage our students in this from engineering to humanities. That's where it's transformational. It's not just being restricted to computer science or engineering. We have students and faculty in digital humanities. We have social scientists and those in bioinformatics, looking at a computing environment of this kind and saying, "OK, how can I bring my problem to this? What is it going to let me do in terms of new levels of creativity that I haven't been able to do before?" That's exciting. And it wouldn't have happened if the machine hadn't been placed in a large public university like Illinois.

Q. Do you see that as a generational thing? An Illinois thing? Something else?

A. I think our students are really forward thinking. I don't know of too many universities whose students have collected additional fees to put into addressing environmental challenges. I don't know of another university where they've actually funded the recycling of food waste.

I say this because I think it's not an accident. We get the best students. The students come here because they've heard of great things happening at centers like NCSA, centers like Beckman Institute or the Coordinated Science Lab. When they come here, they see these opportunities. The word spreads very quickly.

I think all of this makes for the excitement. And I think it's great to see. The investment that we've made and the people that we've nurtured over these years being at the center of this and being so much integrated into the thinking of the campus.

I would say this has been a very wise investment. The return has been tremendous.

Q. You talked about the national and international reputation of places like NCSA and Beckman. How does Illinois make best use of that reputation?

A. The value of these multidisciplinary labs that we have at Illinois is that they are agile. Our departments have to put forward curriculum. They have to really be in the throes of undergraduate education. The departments in my sense are like these big battleships that need to move, but they can't turn as fast.

Q. Great impact though, from a battleship.

A. The impact can be huge. But places like NCSA and [Illinois'] Institute for Genomic Biology and Beckman, they have an agility. They can move into new areas.

The real value to the undergraduate, to the education enterprise, is that when professors are moving into new areas, this material goes into the classrooms. It goes into the graduate classrooms, next semester it goes into the undergraduate classrooms. And that's why our reputation is as high as it is. These labs play a major, major role. Also, it goes without saying that it attracts the best students, it attracts the best faculty.

Q. Tell us how we take advantage of this success to project out to that next thing and to continue to enhance the reputation of the university as a whole.

A. Professors are writing new proposals, and actually advocating new ideas. They are in the front seat in defining what the country should be addressing. We're able to go to [a funding agency like the National Science Foundation] and say, "We know what the country should be doing next." Our faculty, our young faculty and our senior faculty, are very believable when they make this claim.

And if you're defining what the direction should be, then you're in the front seat in receiving that funding.

So it's a whole cycle of faculty leadership, student leadership, and indeed I'd say it is these experiences that make the students go and think in a very entrepreneurial way. They see the faculty as being adventurous, and they start thinking we could start some companies. We are now known as the place where undergraduates go and start big companies and are very successful.

Q. Given some students' past successes—Mosaic, YouTube, PayPal—the entrepreneurism, it seems, has a level of creativity that goes at an angle from what they learn in class.

A. Where I see our students really excel is in out of the box thinking. Beyond the classes they take, it's the peer group. Talking about things outside their research and, of course, the training that we give. It's the rigor of the training. We set high expectations. We expect them to set high expectations of themselves.

So it's that kind of an environment we provide. And I come back to this: The difference between Illinois and big campuses like ours is the existence of these multidisciplinary laboratories where students can really go and think and work and get some experience. It gives them a sense of excitement that they won't get elsewhere. It's what keeps us competitive. I think it's what keeps our country going toward a direction that we continue to be really competitive and creative.

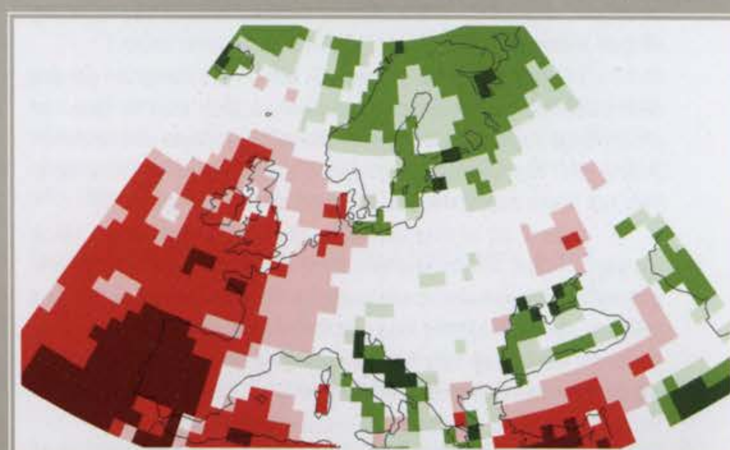
'PEOPLE'S LIVES ARE AFFECTED'

EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS' MODEL OF EUROPEAN PRECIPITATION FOR APRIL TO OCTOBER.

The model shows the expected change in precipitation when the historical average of 1961 to 2007 is compared to the average simulated precipitation for the years 2071 to 2117. The top image is at 128-kilometer resolution, the bottom image is at 16-kilometer resolution. The two simulations produce the same Iberia-Siberia axis of reduced and enhanced rainfall, but the high-resolution simulation has a much larger magnitude change than the low-resolution run. The science team's work as part of the Petascale Computing Resource Allocations program will allow them to conduct high-resolution runs on Blue Waters and make more, and more precise, regional climate predictions like these.

T1279 (16-KM) GROWING SEASON (AMJJASO) PRECIPITATION (% CHANGE)

T159 (128-KM) GROWING SEASON (AMJJASO) PRECIPITATION (% CHANGE)



by J. William Bell

The Blue Waters sustained-petascale supercomputer will help researchers figure out ways to blunt climate change and develop local strategies for living with the changes that do occur.

A SCIENTIFIC CONSENSUS HAS EMERGED: The Earth's climate is changing, and human behavior is accelerating that change.

Climate modeling on supercomputers played a huge role in establishing those facts. It's also being used to guide strategies for blunting the negative impact that climate change will have. Multi-trillion dollar decisions, by the reckoning of the United Kingdom's Office of Climate Change, will be made based on the predictions of our planet's future that can be made by leading scientists using leading-edge supercomputers.

The Blue Waters sustained-petascale system coming to NCSA is likely to be one of the supercomputers delivering those insights—thanks to partners from the Institute of Global Environment and Society's Center for Ocean-Land-Atmosphere Studies (COLA), the University of Miami, the University Corporation for Atmospheric Research, and Colorado State University.

Blue Waters, and world-class supercomputers like it, give these researchers "a place to test ideas and not be fettered by computational constraints," or at least be fettered by fewer constraints, according to Jim Kinter, COLA's director.

Blue Waters' large and fast memory will help researchers get over some of those constraints. Tightly coupled shared-memory nodes will deliver 512 GB/s of aggregate memory bandwidth and 192 GB/s of bandwidth to a hub chip used for I/O, messaging, and switching. The hub chip delivers a total of 1,128 GB/s peak bandwidth.

Blue Waters' large archive—expected to be as much as half an exabyte—will also be important.

"Storage capacity is always a problem" for climate modelers, says COLA's Cristiana Stan. A single run can produce hundreds of

terabytes of data, and the modelers "never destroy the data. We want to be able to analyze it and compare it with past results. We also want to be able to compare it to future generations of models."

As part of the National Science Foundation's Petascale Computing Resource Allocations (PRAC) program, the team is making a broad set of improvements to the Community Climate System Model. This massive computing code combines 3D ocean models, 3D atmospheric models, and 2D surface models that simulate things like vegetation, soil, rivers, and lakes. The Community Climate System Model has been used throughout the climate modeling community for years.

The trillion-dollar question

The improvements are needed because they will allow scientists to refine and improve the models, which are by necessity approximations. "These represent the best we can do, not the best we could do," says Kinter.

Current models provide an excellent view of overall climate. Assessments by the Intergovernmental Panel on Climate Change were based on comparing many of these models, generated by scientists around the world. All had their differences, but all painted the same big picture that the Earth was changing and that things like carbon emissions were impacting that change. The insights from those model-based assessments yielded a Nobel Peace Prize for the panel in 2007.

Current models do not provide accurate predictions of the impact in smaller regions, however.

"Global temperature change of one degree is very different than a particular region changing by three degrees. We know that global precipitation will be reduced, but that tells us nothing about Indian monsoons," observes Stan, who is principal investigator on the team's PRAC award.

"People's lives are affected," she says.

"Children either are or aren't going to be able to take over their parents' wineries in Europe. Droughts either are or aren't going to continue and worsen in western North America," Kinter says. "Our models can't currently tell the difference.

"The trillion-dollar question is how much precipitation and temperature will change and exactly where. We haven't been able to do that at the subcontinent scale."

Simulations on systems like Blue Waters will allow scientists to establish that climate modeling can in fact provide reliable predictions at the regional level. They'll then use those models to develop global strategies for reducing the impact of climate change and more local strategies for living with the changes that do occur.

Heads in the clouds

Improvements to the Community Climate System Model will require better resolution. Current simulations wrap the globe in a grid of cubes 250 to 100 kilometers on each side. With Blue Waters, they hope to get that down to 20 kilometers or smaller on each side.

Inside these cubes, everything from global currents that run thousands of kilometers to the viscosity of centimeter-scale drops of water is simulated. This breadth can produce what are known as "rectified effects." These effects amount to big discrepancies in the climate models that are spawned by the fact that the smallest features of those models aren't being simulated in enough detail.

Rectified effects produce things like an El Niño cycle that you can set your watch by instead of an erratic climate cycle that isn't the same size or intensity every time, as it is in the real world. On the flip side, they make for models that fail to capture the Madden-Julian oscillation, clusters of thunderstorms that plague the tropics of Indonesia.

Abolishing these rectified effects will require treating certain aspects of the models, like clouds and the small eddies that roil the ocean, in fundamentally new ways.

Take clouds, for instance. "You see a little white spot, but, believe it or not, they influence large-scale climate," Stan says. "We need a very high-resolution model of these very small entities."

Today, there's no way to represent clouds at their native scale in global models. Instead, researchers develop and use a statistical representation of the overall impact that clouds have on the climate. "It doesn't work as well as it should," Kinter says.

Even with Blue Waters and its generation of supercomputers, they won't be able to model individual clouds at the one-kilometer scale that they require. They will, however, apply a technique called "superparameterization." This will allow them to model hundreds of clouds in a given grid region and aggregate the impact of those for that section of the model. "Now that's extremely effective, and it has been shown to work much better than the old way," Kinter says.

With that method in place on Blue Waters, the team hopes to run the first global cloud-resolving model for the United States and to integrate the results into global climate models, too.

"That model, we will call a very big victory," Stan says. □

PROJECT AT A GLANCE

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Benjamin Kirtman
William Large
David Randall
Cristiana Stan

FUNDING

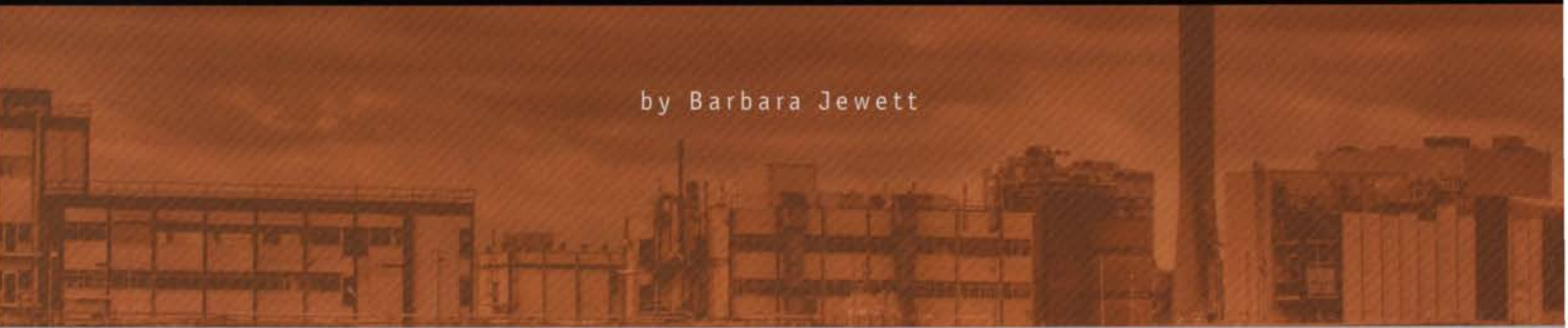
National Science Foundation

FOR MORE INFORMATION

www.iges.org/cola.html
www.hm-treasury.gov.uk/stern_review_report.htm

ACCESS ONLINE

www.ncsa.illinois.edu/News/Stories/climate



by Barbara Jewett

THE INDUSTRIAL CONNECTION

POTATO CHIPS that stay on conveyor belts instead of flying around the manufacturing plant. Energy efficient diesel engines. Safer pesticides. Environmentally friendly product packaging. New cell phone technologies. Better airplane wings. Improved pharmaceuticals. These are just a few of the areas supercomputers have assisted manufacturers in improving products while cutting costs.

But industry's demand for, and use of, high-quality science and engineering is not well documented, says Merle Giles, director of NCSA's Private Sector Program (PSP). In some instances it is not even well understood. That's why Giles and the PSP are excited to help lead the way in documenting and improving the use of science by the industrial computational community through two new projects.

EAGER award

One project is already underway. With a $200,000 EArly Concept Grant for Exploratory Research (EAGER) award from the National Science Foundation, Giles and his team are documenting the use of science by the industrial computational community. They expect to aid understanding of the interplay between federally supported university-based research and industrial research and development, highlighting how interdependent academic and industrial science are. The project will also relate high-performance computing (HPC) efforts within large U.S. companies to university-based research, identify use cases that drive industry demand for high-quality research, and identify practices that could potentially foster alliances in advanced software development, including petascale computing. In addition, they hope to link to activities at a number of federal agencies and departments.

Industry demand for simulation-based engineering and science has increased due to a variety of factors, explains Giles. Companies face economic pressure to decrease time-to-market. They also need to utilize multi-disciplinary physics to address product complexity and safety, and have a general inability to conduct physical prototyping due to miniaturization, complex materials manipulation, or safety. In addition, companies want to take advantage of modern production methods and energy innovation and conservation.

"The capability of high-performance computing to run models with high fidelity and physical accuracy is of great interest and great benefit to these companies," he says.

Midwest project

Small and medium sized manufacturing enterprises (SMEs) in the United States rarely use modeling, simulation, and analysis. Studies by the Council on Competitiveness and others show that the barriers to entry are resource driven; in particular, a lack of a support network and internal expertise to move up the learning curve. On March 2, The Midwest Project for SME–OEM Use of Modeling and Simulation was launched at a signing ceremony in Washington, D.C. The project is part of the National Digital Engineering and Manufacturing Consortium (NDEMC) that is being developed for the purposes of promoting adoption and advancement of modeling, simulation, and analysis in U.S. manufacturing and the related supply chain.

NCSA and private corporations are partnering with the Economic Development Administration (an agency within the U.S. Department of Commerce) and non-governmental organizations in a nearly $5 million effort to provide education, training, and access to supercomputing resources so that SMEs can develop modeling and simulation skills.

"This is a large-scale, public-private partnership," says Giles. "Private companies are putting up most of that money and it has the attention and involvement of a U.S. agency not previously involved with high-performance computing. That's exciting for the HPC community, especially those of us who work with the private sector."

NCSA will provide trainers and domain experts to train staff at select companies in HPC, modeling, and simulation.

Other project partners include the Ohio Supercomputing Center, the Council on Competitiveness, the National Center for Manufacturing Sciences, and Purdue University. Industrial partners are Deere & Co., General Electric, Procter & Gamble, and Lockheed Martin.

"Most of the companies involved are NCSA PSP partners," notes Giles. "We already have relationships with those companies, so that will allow us to get up to speed quickly on this project."

Through the NDEMC and the Midwest project, collaborators look forward to accelerating innovation through the use of advanced technology. The goal is greater productivity and profits for all players through an increase of manufacturing jobs remaining in and coming back to the U.S., and increases in United States exports. □

Medium

SPACE IS NOT EMPTY. In fact, says Zhibo Yang, there's an area of the universe called the interstellar medium (ISM) that is filled with molecules, atoms, ions, and grains of dust. And these things are conducting some very interesting chemical activity.

Ion-molecule reactions are dominant among these reactions. Yang, a post-doctoral researcher at the University of Colorado, Boulder, and his colleagues are studying reactions that involve negative ions with the help of the Abe supercomputer at NCSA.

"Positive ions have been relatively well studied," says Yang. "But negative ions have only recently been detected in the ISM."

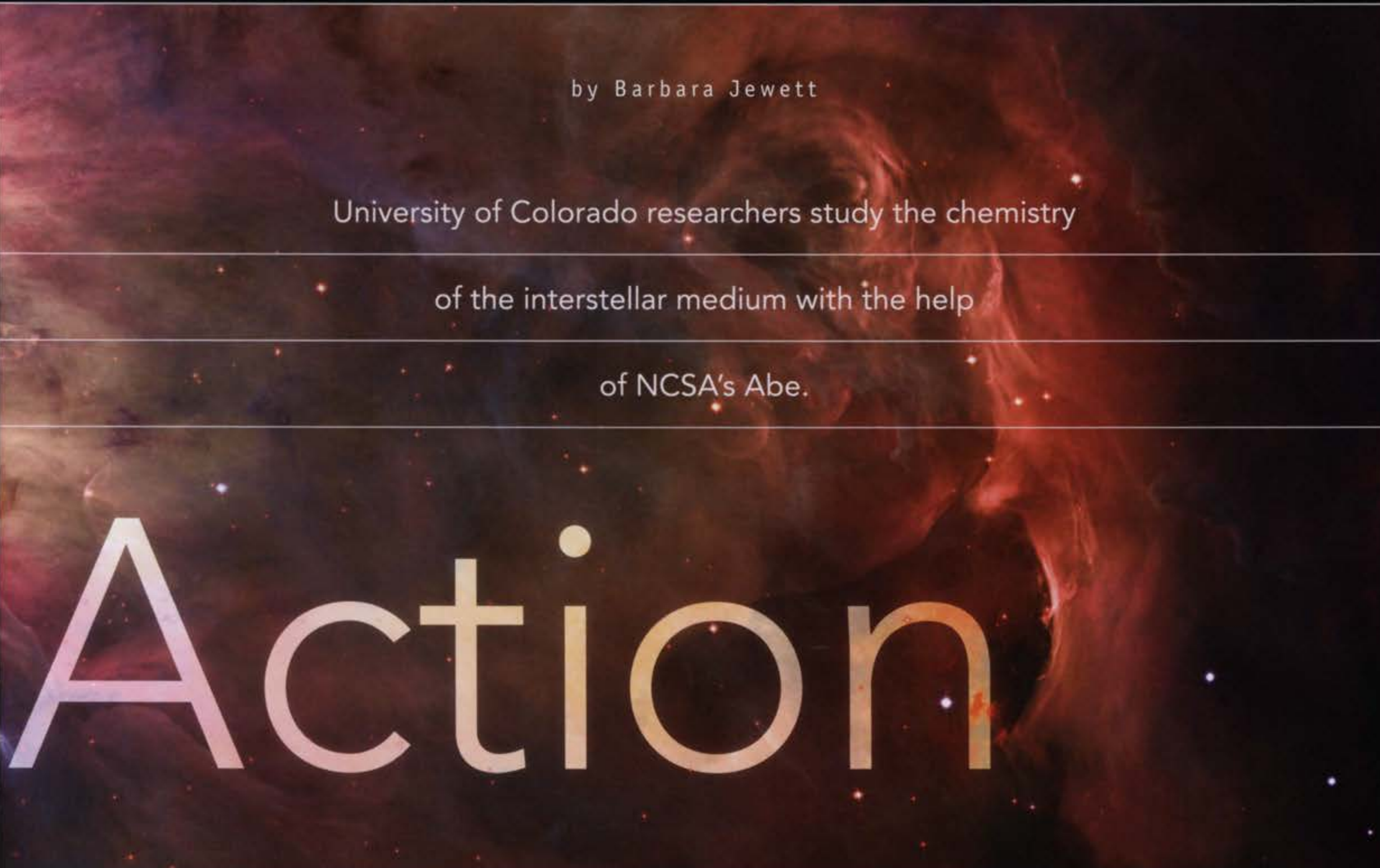
More than 160 molecular species have been detected in the ISM. And evidence is mounting, he says, in support of the existence of large organic species such as polycyclic aromatic hydrocarbons (PAH). But little is known about the chemical origins of these species. A complete understanding of the evolution and interconversion of species in the ISM will require detailed data on the chemical and physical processes occurring throughout space.

Yang's team is looking at the reaction between ions and neutrals, measuring the rate constants of these reactions, and the mass to charge ratio of the negative ions using mass spectrometry. But mass spectrometry yields no information regarding the ion structure. To get information about the structures and energies and to understand their reactivity requires calculations. Very large calculations.

"In principle, some small calculations can be run on our PCs, but for the large calculations we can not affordably carry them out on our PCs. Also, our PCs do not have enough memory, they crash with the large calculations," explains Yang. "The typical calculation will last for 12 hours on our PC but we can do the same calculation on Abe in about two to three hours."

So far, the group has completed both experimental and theoretical studies of reactions between atomic species (i.e., hydrogen, nitrogen, and oxygen) and anions (i.e., carbon chain anions and some typical molecular anions). Five oral presentations have been made at international and domestic conferences and six papers were published in 2010, in the *Journal of the American Chemical Society*, the *Astrophysical Journal*, and in *Physical Chemistry Chemical Physics*.

While the team does some experimental work, Yang says the low temperatures of the ISM and the diverse pressures usually cannot be replicated in a laboratory setting. In a computer simulation, however, researchers can easily set the temperature and pressure. The



by Barbara Jewett

University of Colorado researchers study the chemistry of the interstellar medium with the help of NCSA's Abe.

Action

simulations verify experimental results, and the team's computational work can also help predict the possibility of undiscovered species. And they are providing some fundamental science, general rules to help scientists understand other related reactions.

There are other scientists who are doing modeling, explains Yang, and they want to use the reactions with rate constants in their models. Rate constants are important for astrochemical modeling to establish the reaction networks among species in the ISM. If they can determine when reactions occurred, eventually scientists can predict the evolution of the universe.

While the team's current research may seem esoteric, he notes, other scientists use the results for their research projects that are likely to draw more public attention. But the team's research successes are helping their careers. Yang says he's had several interviews in his quest to secure an assistant professorship and one PhD student just finished his thesis defense and has a position at Harvard for postdoctoral research.

When settled at a new university, Yang hopes to do studies in other areas that will attract more public attention, such as biomolecules, catalytic reactions, and renewable energy. With the help of NCSA, of course. □

PROJECT AT A GLANCE

TEAM MEMBERS

Veronica M. Bierbaum
Theodore P. Snow
Zhibo Yang
Callie A. Cole
Nicholas J. Demarais
John M. Garver
Oscar Martinez Jr.
Charles Nichols
Marshall Carpenter
Denver Hager

FUNDING

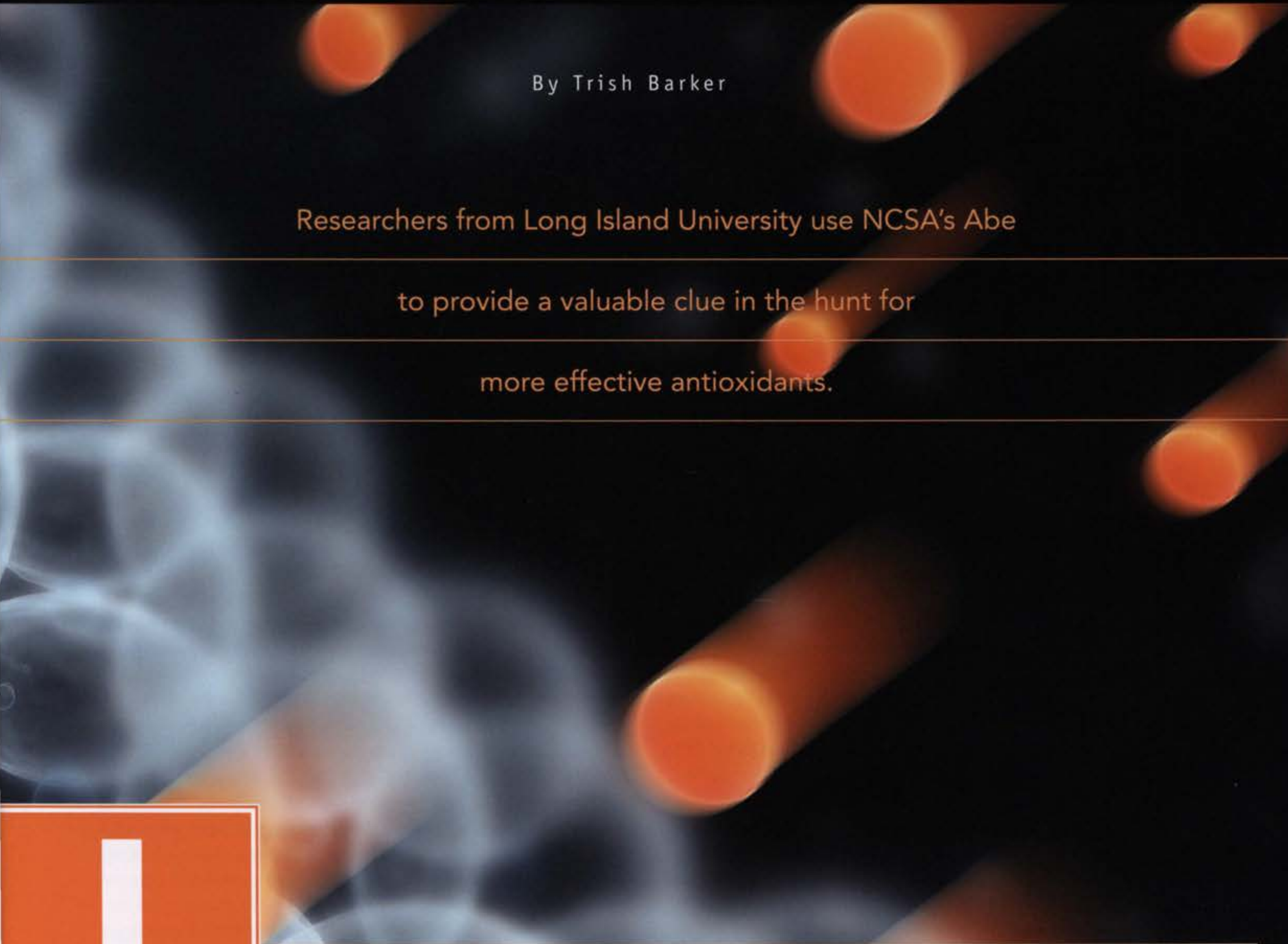
National Science Foundation
NASA

ACCESS ONLINE

www.ncsa.illinois.edu/News/Stories/medium

FREE RADICALS

—Get them before they get you!



By Trish Barker

Researchers from Long Island University use NCSA's Abe to provide a valuable clue in the hunt for more effective antioxidants.

IN THE 1970S, Andreas Zavitsas had a theory that the key factor determining the rate of free radical reactions was the starting energy of the reactant, or parent, molecule. But other scientists, and their data, suggested that the variations of stabilities of transition states were most significant in determining reaction rate. And for about four decades, Zavitsas lacked the necessary computer power to carry out the demanding quantum mechanical calculations that could demonstrate whether his theory was correct.

Then came Abe. At last, Zavitsas and his colleagues in the Department of Chemistry and Biochemistry at Long Island University, Donald Rogers and Nikita Matsunaga, were able to show that variations in the ground state stabilities of the reactants can be as important in controlling how fast a chemical reaction proceeds. Their results were published in *The Journal of Physical Chemistry A* in October 2009.

"We are so appreciative that centers such as NCSA exist," Matsunaga says. "We run a relatively small research lab. It's very important for us to have access to computers such as Abe; it really changes how we do our research here."

Radicals, ready to react

Because they have unpaired electrons, free radicals are highly reactive loose cannons, capable of playing beneficial roles in important industrial processes, like combustion and polymerization, but also of causing cell damage in our bodies. That damage is linked to aging and disease, including Parkinson's, diabetes, and cancer.

"When a free radical reacts with a molecule, it forms another free radical, which reacts with another molecule to produce another free radical, and so on and on," explains Zavitsas.

"The same process keeps going around and around in a circle, a chain reaction, producing these free radicals. Which in abundance cause damage," says Rogers.

Tocopherols (which most non-chemists know as vitamin E) can dead-end that damaging chain reaction by quickly reacting with the original free radical to form a stable free radical that refuses to react and breaks the chain.

"We know experimentally that vitamin E is very good at trapping free radicals in the body," Zavitsas says. "They are good because

Nikita Matsunaga, Donald Rogers, Andreas Zavitsas

they react with chain radicals very, very fast. And why vitamin E reacts with free radicals so fast goes back to the rate of reactions."

The question of what controls the speed of the radical reactions has been lingering for around 40 years, he says.

"We know that the reaction of vitamin E with chain radicals is very fast, but it is not clear that we understand why it's as fast as it is," Rogers says. "And that's very important, particularly in biological systems, because...the molecule that crosses the finish line is going to be the final product. The chain reaction that is carrying out a process that is implicated in carcinogenesis and in cell damage, if that is faster than the reaction of so-called sweepers (the tocopherols that make up vitamin E for example), you essentially have a kind of a race between the vitamin E and the free radicals. Which of those reactions wins out is the determining factor as to whether you're safe or unsafe."

The top of the hill is half the story

For years, in trying to understand the factors affecting chemical reactivities, chemists had focused on variations of stabilities of transition states, the short-lived species atop the energy hill between reactants and products.

"People have focused in general on the height of the energy hill and on the structure of the molecules that are reacting on top of the hill," Zavitsas says. "We have suggested that one shouldn't only look at the structure at the top of the hill, but also look at the structure of what you're starting with."

The Long Island researchers examined benzyl fluoride with 11 common substituent groups in the meta and para positions; substituent groups are the atoms, or groups of atoms, that hang onto a hydrocarbon chain (in this case, a benzene ring) in place of a hydrogen atom, and para and meta are different positions where they can hang. They wanted to see how electron-donating and electron-withdrawing substitutents influenced the ground state molecular stabilization energy of the benzyl fluoride molecule and hence the activation barrier of benzylic fluorine atom abstraction by free radicals.

"We were interested in comparing the enthalpies [heat transfers] of benzylic molecules, which had very negative species attached to one end to those which had a very positive species attached to one end," Rogers says. "What we wanted to do was find out how the negativity or positivity influenced the energy of the molecule."

Using the G3 and G3(MP2) model programs on NCSA's Abe supercomputer, the researchers calculated the energies of the ground state and free radical transition state for benzylic abstractions from the 11 selected molecules.

"In order to calculate these very large energies, it takes a lot of computer time. And your computed results need to be very accurate, because you are looking for minute differences," Rogers says.

"It's like trying to get the weight of a captain of a superliner by weighing the superliner with and without the captain aboard," Zavitsas adds. "And these supercomputers make this possible. Just a few years ago, one couldn't do this at all."

"[Abe] is stupendously fast," Rogers says. "It's the fastest machine I could get my hands on! Any time you guys come up with a faster one, I'd like to get time on it!"

In addition to access to computing time, support for their research comes from the Whiteley Foundation and Friday Harbor Laboratories, University of Washington, which contributed research time and facilities. Their work is also supported by the Intramural Research Program of Long Island University.

Their calculations showed a strong correlation between the substituent's electron-withdrawing or -donating properties and the energy of the parent molecules, as measured by independent experimental methods.

"We found that the energy patterns fit very well with the rate patterns or the speed of reaction," Rogers says. "If you plot speed of reaction for this series of 11 molecules, and the energy of the ground state, you find that the patterns look almost identical. This leads to the conclusion that the rate of the reaction is predominantly determined by the energy of the reactant molecule."

Their conclusion is that when it comes to determining reaction rates, a narrow focus on the transition states without attention to the ground state stability tells only half of the story. "Our work demonstrated that variations in the stabilities of the reactants can be as important in controlling how fast a chemical reaction proceeds," Rogers says.

Zavitsas says this reaction rate knowledge will be significant for researchers who are trying to make better free radical blockers. "Using knowledge about what controls the rate of free radical traps is the basis for trying to get something better." □

PROJECT AT A GLANCE

TEAM MEMBERS

Donald Rogers
Andreas Zavitsas
Nikita Matsunaga

FUNDING

Whiteley Foundation, University of Washington
Long Island University

ACCESS ONLINE

www.ncsa.illinois.edu/news/Stories/radical by Allison Copenbarger

GREEN MACHINE

WITH GUIDANCE FROM PROFESSORS and experts at NCSA, students got hands-on experience building their own supercomputer with NVIDIA graphics-processing units. Their system took third place on the Green500 list in November 2010 and was named the greenest self-built cluster.

For Tyler Takeshita, helping to construct a supercomputer was like meeting a familiar friend in-person for the first time. Takeshita, a graduate student in chemistry at the University of Illinois, has been interested in computers since a young age and belongs to a computational research group led by chemistry professor (and NCSA director) Thom Dunning.

"It was very helpful to get hands-on experience," Takeshita said. "It was almost like putting a face to the name when you have an idea of what things look like and how they fit together."

Takeshita, along with around 15 other students, participated in building a supercomputer to enter into the Green500 competition—a ranking of the most energy-efficient supercomputers in the world. The project was part of an independent study course led by Bill Gropp, professor of computer science and a co-principal investigator on the Blue Waters project, and Wen-mei Hwu, professor of electrical and computer engineering and also a Blue Waters co-PI. Mike Showerman and others at NCSA provided cluster-building expertise and assistance.

"The idea is kind of original because it's not trying to use a big machine that consumes a lot of energy to be really fast," computer science major Chengyin Liu said. "We were interested in efficient power consuming. I found the idea very interesting."

According to Showerman, the first step was selecting the perfect equipment. In this case, that was NVIDIA's C2050 graphics-processing unit (GPU). While GPUs were originally developed to render graphics, today they are being adopted as computational accelerators; with the proper software adaptations, some codes can run substantially faster using GPUs' many-core architecture. Even as the students were building their cluster, China announced that their GPU-CPU hybrid machine, Tianhe-IA, would move to the number one spot on the Top500 list.

NVIDIA donated 128 C2050 units to the Illinois CUDA Center of Excellence, led by Hwu, and NVIDIA research scientist Sean Treichler spent time on campus helping to plan and build the cluster. QLogic also donated a portion of the cluster's interconnect.

Treichler noted the students had some good ideas when it came to connecting components in a creative way. To save money and reduce the cluster's footprint, the team used nontraditional materials, like wood and Plexiglass, to mount the motherboards.

The students had three big sessions working tirelessly in the new National Petascale Computing Facility to build the cluster, which they named EcoG. They also needed to configure all of the settings and check each memory card, processor and cable for problems before finally running benchmark code to test their cluster's performance and another test to gather power-usage data by their deadline. Finally, the team recorded performance of 33.6 teraflops (or 33.6 trillion calculations per second) and 938 megaflops per watt.

The cluster landed spot 403 on the Top500 list and then took third place when the Green500 was posted on November 18, 2010. EcoG won an additional Green500 honor as the "greenest self-built supercomputer."

Showerman feels the project was a success and says Illinois will likely continue to have cluster-building classes in coming years as the combination of book knowledge and hands-on experience has merit.

"We used the cluster to conduct studies on how real applications may need to be adapted to run well on such power-constrained systems," says Hwu. "This will likely be the norm in exascale computers in the next decade." □

PROJECT AT A GLANCE

TEAM MEMBERS

- Jeremy Enos
- Bill Gropp
- Andres Guzman-Ballen
- Wen-mei Hwu
- Forrest Iandola
- Danny Johnson
- Matt Johnson
- Chengyin Liu
- Gregory Meyer
- Nady Obeid
- Abhishek Pradhan
- Lucas Scharf
- Mike Showerman
- Craig Steffen
- Tyler Takeshita
- Felix Wang
- Lu Xu

BEHIND THE SCENES OF NCSA

MISSION:

Above: Mike Dopheide, security engineer, Brad Sheafe, cybersecurity deputy director/chief security officer, Tim Brooks, security engineer, Jim Barlow, head of security operations and incident response.

THOUGH THEY'RE NOT QUITE AS CLANDESTINE as an impossible missions force, the work of NCSA's security operations team is just as vital and nearly as challenging. This group of network security specialists supports the center by applying the latest cybersecurity advances to protect NCSA's high-performance computing resources. They also maintain the integrity of staff computers and networks.

In close collaboration with other NCSA groups, the security operations team of Brad Sheafe, Jim Barlow, Mike Dopheide, and Tim Brooks focuses on assessing, detecting, and mitigating the risks to networks and computational systems. By applying technology and applications in various areas to strengthen the center's overall security posture, they provide a balance between security and usability. This ensures that the center's mission—operating some of the world's most powerful supercomputers and developing the software infrastructure to efficiently use them—is met. The team helps everyone at the center become more security aware by providing training and education sessions, and they assist staff members and users who are having security-related issues.

"At NCSA, network security is a high priority and our team's efforts are viewed as a good thing," says Jim Barlow, head of security operations and incident response. "And when you have team members who are approachable, are well-liked, and have a sense of humor the way ours do, it makes the cybersecurity job a little

SECURITY

easier as people will work with you by following your advice. Most importantly, people let us know when they think something is not right so that we can investigate."

Thanks to the efforts of this team, NCSA users and staff can login with confidence that their data and communications are secure. □

1986 25 2011

by Barbara Jewett

GOING SOMEWHERE

NCSA TURNED 25 IN JANUARY. Bob Wilhelmson was at NCSA from the very beginning. Although he formally retired last year, he still is involved with the center. When the unsolicited proposal that gave birth to NCSA was written and sent to the National Science Foundation (NSF) in 1983, high-performance computing was being discussed by folks at NSF and in the research community, says Wilhelmson, but he and the other co-principal investigators on the proposal led by Larry Smarr "thought we'd move things along a bit."

That decision to move the discussion to its logical conclusion greatly impacted Wilhelmson's work as an atmospheric scientist at the University of Illinois. Like many campus researchers at the time, he needed to travel to the National Center for Atmospheric Research (NCAR) in Colorado to use its large computing systems. Or he'd submit jobs to NCAR via telephone modems and punched cards and then wait for output in the mail. Some researchers on campus were even traveling to Germany to do their computing. To them, that just didn't make sense.

Wilhelmson studies severe storms, looking, for example, at supercells (strong persistent storms), which produce the strongest tornadoes. When Blue Waters comes online, he believes he will finally be able to simulate these storms and any embedded tornadoes with enough fidelity to capture what is happening at the smallest scales within the storm and around the tornado that influence tornado genesis, evolution, and decay. Atmospheric scientists currently cannot do this.

"And when we do that, we're not only simulating the tornado but we're simulating the whole storm with high fidelity. How the storm behaves as a whole also influences what is happening on the ground in terms of high winds, tornado structure and strength, and damaging hail," he explains.

In the beginning . . .

Simulations, even in the early days, produced lots of data that needed to be analyzed and visualized. Wilhelmson says that he would create two-dimensional contour plots of his NCAR data that were written to microfilm and mailed to him if he was at Illinois.

"Nobody even thinks of that today," he laughs. "Decisions were made early on that we were going to do things a little differently at NCSA. We needed new and faster ways."

This included animating the data using software developed at NCSA. In addition, new ways were developed to communicate scientific results to other researchers and the public. NCSA brought in people from the West Coast who were developing software and animations for commercials and movies. This has led to productions shown in planetariums, in museums, and visualizations in 2D and 3D IMAX films and television documentaries.

"Our thought was, why can't we use what they are doing and apply it to the data that we're producing on our supercomputers. And that's how we proceeded. Software was developed here and when coupled with high-end visualization software in use on the West Coast helped to lead the revolution in scientific visualization at the time. Further, there was a marrying of computing technology on the very large high-performance scale and the computing technology on one's desktop so that you could actually see and animate these visualizations on a computer screen in three spatial dimensions and time," says Wilhelmson.

Digital visualization of data produced during a simulation impacted his research. His team already had millions of pieces of data, "and then all of sudden computers get faster and there's billions and trillions of pieces of data we're trying to make sense of, both in terms of structure of storms and storm evolution." What

was exciting about NCSA's approach, he says, was that he could see renderings of the data no matter what its size, and ask questions about it that could be answered quickly with new animations. Today, researchers carry out simulations and produce visual animations directly from the simulation data, which is made available through web browsers.

"When we started, there was this 'I wonder where we're goin', but I know we're not stayin' where we're at. We're goin' somewhere.' That was before Facebook, before the Internet as we know it today," says Wilhelmson. "There was an excitement when we started because we were all packed together in a building, we were young, we had dreams of what we wanted to do, and what NCSA as an organization should be."

The university and NSF didn't know NCSA was going to be a highly recognized organization 25 years later, he says, but they provided the backing and Illinois had the leadership and the scientists on campus who could carry the idea forward.

"The capability of NCSA is rooted not so much in the hardware, that changes every few years, but in its people," says Wilhelmson. "It is taking innovative ideas and developing them so that the end user can carry out their research more effectively and answer questions that they only dreamed of answering a few years before."

USER REFLECTIONS

MICHAEL NORMAN

University of California, San Diego

[Editor's note: Michael Norman, director of the San Diego Supercomputer Center, was, until 2000, an astronomy professor at the University of Illinois and an associate director and senior research scientist at NCSA.]

Preparations for observing NCSA's 25th anniversary this year revealed several users who computed at NCSA in 1986 who are still active users today. We invited them to share their thoughts on advances in high-performance computing.

Q. What were you studying when you used NCSA's first supercomputer, the Cray X-MP? What new results came from its use? What other NCSA capabilities helped you advance your science?

A. I was studying the structure and dynamics of extragalactic jets using 2D supersonic gas dynamic simulations. Using the X-MP, I was able to simulate considerably larger domains at high resolution and examine non-axisymmetric (firehose) instabilities. I worked with Donna Cox's visualization group to make striking animations of the instabilities, which elucidated the dynamics in a beautiful and informative way.

Q. In what ways has access to supercomputers at NCSA advanced your science since then?

A. Countless ways. Between 1986 and 2000, when I left NCSA, I used everything NCSA put on the floor to increase the physics fidelity of my extragalactic jet simulations. The Cray-2 and Connection Machine-2 allowed me to go to 3D simulations, and eventually incorporate magnetic fields. The Connection Machine-5 deployed in 1992 launched my research on cosmological structure formation, which continues to this day. The SGI clusters in the mid to late 1990s provided an ideal platform for developing the Enzo adaptive mesh refinement code for hydrodynamic cosmology, which is my main research tool today. Since 2000 I have used many NCSA resources to study galaxy clusters, the intergalactic medium, the formation of the first stars, and interstellar turbulence.

Q. In what areas do you envision advances in supercomputing capability having the most impact in your research during the coming 5–10 years?

A. Blue Waters will take my numerical cosmology research to the next level. Multiphysics AMR simulations of star and galaxy formation are very compute intensive; the speed and number of POWER7 processors that will be available will enable high-fidelity simulations of the formation of the first galaxies and reionization. We are already drowning in the data volumes current generation supercomputers produce. Data-intensive computer architectures with large amounts of shared memory and flash SSD will be ideal data analytics platforms. HPC systems with more productive parallel programming languages and tools would also have a big impact.

Q. Is there anything supercomputers enabled you to do 20-25 years ago that you thought was really 'wow' and cutting-edge at the time, but that you look back at now and smile at the memory of how 'high tech' you thought you were at the time?

A. Yes. The transition from NCSA's Cray Y-MP to the Cray-2 was a "wow" moment for me. Its large memory (128 MW!) allowed me to move from 2D to 3D simulations of extragalactic radio jets—from cartoonish flatland models to astrophysically realistic-looking models. The Cray-2 stimulated the development of the ZEUS-3D code in my lab from 1989 to 1992. ZEUS-3D went on to be the first open-source community code in astrophysics, and it is still in use around the world. At the time, around 1988, I remember being quoted in the local paper saying that trying to fit a 3D simulation into the YMP's memory was like fitting an elephant into a tutu. That quote made it into the quotes of the week. That makes me smile when I think of it.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NCSA HONORS

STAFF RECOGNITION AWARD WINNERS

NCSA EMPLOYEES recently gathered to celebrate the center's successes and honor colleagues' innovative ideas and dedication to NCSA. A few of the remarkable people at NCSA were honored with staff recognition awards for 2010 for their outstanding contributions to NCSA's core mission of driving science and engineering through high-performance computing. In addition to a certificate, honorees received a $500 individual award and a $500 award for each recipient of a group award (up to a $2,000 maximum award).

Administrative Excellence

Doug Fein[5]

As leader of NCSA's Information Technology Services, Doug continually learns new ways to apply advanced IT solutions to NCSA's challenges while focusing on two goals he set for his team: drive down IT costs and improve customer service to NCSA staff. When asked to streamline server costs, he was able to reduce 16 racks/65 servers to four racks/16 servers, improving service and uptime in the process. Other units on campus often seek his advice and expertise.

Best Technical Achievement: Automated Learning Group

Bernie A'cs[3], Loretta Auvil[1], Boris Capitanu[11], Michael Haberman[9], and David Tcheng[7]

This team's dedication, collaboration and drive was put into developing the tools SEASR and Meandre, which scholars in any discipline can adapt for data-driven knowledge discovery. In doing so, they engaged two very different communities—the tool builders in information and computational science and researchers/scholars—in a dialogue, thus going beyond just providing software to helping build a community to assist researchers in gaining proficiency with data-driven applications.

Best Collaborative Effort: Private Sector Program team

Evan Burness[4], Seid Koric[2], Luke Scharf[8], and Ahmed Taha[6]

PSP has relied on close collaboration over the last year, both internally and with partner organizations, to improve service to the American industrial community. The team has relentlessly pushed the boundaries of NCSA's Abe and Ember clusters, as well as other TeraGrid resources, to cultivate unmatched insight into the ideal pairings of hardware and software for high-performance industrial applications. In turn, PSP has leveraged this expertise to advance partner interests, bring attention to university research efforts, and offer compelling development environments. The team has been lauded by a variety of organizations for its outstanding customer service and flexible partnerships that surpass alternatives from other public and private HPC providers.

Best Team Player

Cristina Beldica[12] and Brett Bode[10] (tie)

Two key members of the Blue Waters project are both being honored as Best Team Player—a tie is clearly a sign of strong teamwork!

As the senior project manager for Blue Waters, Cristina serves as the "go-to" person when any project participant needs guidance. She oversees all aspects of the project, both day-to-day work efforts and long-term project planning. Her experience in project management, her dedication to the project, and her ability to provide leadership in all areas have been instrumental to the project—internal and external project members all rely on her guidance and information.

As a technical program manager for Blue Waters, Brett works with many diverse members of the team on a regular basis. He willingly steps up and takes a leadership role in multiple areas (often upon short notice), including assisting teams outside his primary duties. Brett is also a member of a success PRAC team and leads a project that received a DOE INCITE grant.

Civil Service Years of Service Awards

Three civil service employees were also recognized for achieving years of service milestones at the University of Illinois. They were:

15 years: Amber Moore
20 years: Vicki Halberstadt
30 years: Beth McKown □

RESEARCHERS TO DEVELOP CYBERGIS

The National Science Foundation awarded $4.4 million to an initiative led by the University of Illinois that will combine cyberinfrastructure, spatial analysis and modeling, and geographic information science to form a collaborative software framework encompassing many research fields.

Led by Shaowen Wang, a professor of geography and also a senior research scientist at NCSA, an interdisciplinary team of researchers will work to develop CyberGIS, a comprehensive software framework that will harness the power of cyberinfrastructure for geographic information systems (GIS) and associated applications. Computer science professor Marc Snir chairs the project steering committee.

The overarching project goal is to establish CyberGIS as a fundamentally new software framework encompassing a seamless integration of cyberinfrastructure, GIS, and spatial analysis and modeling capabilities. Wang says it could lead to widespread scientific breakthroughs that have broad societal impacts, such as disaster preparedness and response or impacts of global climate change.

The project is part of NSF's Software Infrastructure for Sustained Innovation program, which aims to promote scalable, sustainable, open-source software elements. In addition to the advanced problem-solving capabilities, the researchers hope that CyberGIS will enhance sharing among researchers and facilitate cross-disciplinary interaction through multiple-user, online collaboration.

Partner institutions include Arizona State University, the Computer Network Center of the Chinese Academy of Sciences, Environmental Systems Research Institute, Georgia Institute of Technology, Oak Ridge National Laboratory, University College London Centre for Advanced Spatial Analysis (England), University Consortium for Geographic Information Science, University of California-San Diego, University of California-Santa Barbara, University of Washington, the U.S. Geological Survey, and Victorian Partnership for Advanced Computing (Australia).

ADM JOINS NCSA PRIVATE SECTOR PROGRAM

Archer Daniels Midland Company, the global agricultural processing company headquartered in Decatur, Illinois, is the latest Fortune 50 company to join NCSA's Private Sector Program (PSP). The partnership brings together both basic and applied researchers from the University of Illinois campus and beyond, says Merle Giles, PSP director.

PSP puts NCSA's expertise and technological innovation to work on the real-world challenges faced by business and industry. Some of the world's leading companies have leveraged NCSA tools and technologies to gain competitive advantage. Current partners include: Boeing, Caterpillar, John Deere, GE, Motorola, Procter & Gamble, and Rolls-Royce. For more information, go to industry.ncsa.illinois.edu, or contact Merle Giles: mgiles@ncsa.illinois.edu or 217-244-4629.

BLUE WATERS EFFORTS EARN AWARDS AT SC10

NCSA staff, Blue Waters collaborators, and Blue Waters undergraduate interns all took home awards from the SC10 conference.

Torsten Hoefler, who leads performance modeling and simulation efforts for the Blue Waters sustained-petaflop supercomputer project, earned the SC10 best technical paper award for "Characterizing the Influence of System Noise on Large-Scale Applications by Simulation." This analysis of the impact of system noise on large-scale parallel application performance in realistic settings was co-authored by Timo Schneider and Andrew Lumsdaine at Indiana University. The full article can be downloaded at: **http://www.unixer.de/publications/index.php?pub=108.**

A team of undergraduate students, four of whom participated in the Blue Waters Undergraduate Petascale Education Program, won the SC10 Education Program's student programming contest. The nine participating teams had to solve questions in physics, biology, mathematics and computer science, and system benchmarking. The winning team included Ivan Babic (Earlham College), Ben Cousins (Clemson University), Leon Durivage (Winona State University), Brandon Holt (University of Wisconsin-Eau Claire), and Daniel Gerbig (University of Minnesota-Twin Cities).

And at the co-located 3rd IEEE Workshop on Many-Task Computing on Grids and Supercomputers (MTAGS10) the best paper award went to a team of Blue Waters collaborators from the University of Chicago and Argonne National Laboratory—Timothy G. Armstrong, Zhao Zhang, Daniel S. Katz, Michael Wilde, and Ian T. Foster—for "Scheduling Many-Task Workloads on Supercomputers: Dealing with Trailing Tasks."

MORE PRAC TEAMS ANNOUNCED

Five research teams involving scientists and engineers from across the United States were recently given Petascale Resource Allocation (PRAC) awards. They join the 18 teams previously announced. PRAC awards provide allocations or provisional allocations of computing time on Blue Waters as well as travel funds to enable the approved research teams to work closely with the Blue Waters project team at NCSA to tune and optimize their science and engineering applications to take full advantage of the capabilities of Blue Waters. The newest projects to receive PRAC awards are listed below.

- **Hierarchical molecular dynamics sampling for assessing pathways and free energies of RNA catalysis, ligand binding, and conformational change**
  Principal Investigators: Thomas Cheatham, University of Utah; Darrin York, Rutgers; Carlos Simmerling, State University of New York at Stony Brook; Adrian Roitberg, University of Florida; Ross Walker, San Diego Supercomputer Center
- **Petascale multiscale simulations of biomolecular systems**
  Principal Investigators: Gregory Voth and Benoit Roux, University of Chicago
- **Petascale plasma physics simulations using PIC codes**
  Principal Investigator: Warren Mori, University of California-Los Angeles
- **Type Ia Supernovae**
  Principal Investigators: Stanford Woosley, University of California Observatories; Michael Zingale, State University of New York (SUNY) Stony Brook; John Bell
- **Enabling breakthrough kinetic simulations of the magnetosphere via petascale computing**
  Principal investigators: Homayoun Karimabadi, Kevin Quest, Amitava Majumdar, University of California-San Diego

GUIDE TO BEING A 'JOYFUL PROFESSOR'

Barbara Minsker, a professor of civil and environmental engineering at the University of Illinois at Urbana-Champaign and a frequent NCSA collaborator, provides simple-to-follow guidelines for fellow academics to achieve success, rather than stress, in her new book, "The Joyful Professor: How to Shift From Surviving to Thriving in the Faculty Life" (MavenMark Books). By following the guidelines in her book, Minsker says she was able to realign her priorities, reduce her stress, and better balance work and life, thus allowing her time for activities she enjoys, such as canyoneering with her teenage son.

In an essay published Sept. 17, 2010, by Inside Higher Ed, Minsker describes how she learned to better align her activities with her goals and how she seeks to help others do the same through her book and her non-profit organization, Joyful U, Inc., which offers retreats and workshops. More information on these events, the book, and a link to the essay is available at: **www.joyful-professor.com.**

NCSA VISUALIZATIONS HELP TELL 'LIFE: A COSMIC STORY'

How did life on Earth begin? This tantalizing question forms the basis of "Life: A Cosmic Story," which premiered Nov. 6, 2010, at the Morrison Planetarium at the California Academy of Sciences in San Francisco. This all-digital production, produced by the California Academy of Sciences, features a scene created by NCSA's Advanced Visualization Laboratory (AVL).

The AVL team integrated scientific simulations and observed data sets to create a two-minute voyage into the Milky Way galaxy to see the early stages of our solar system before the Earth was formed 5 billion years ago. Viewers fly though lanes of gas and dust into a turbulent molecular cloud where our newly formed sun is accreting a protoplanetary disk prior to the formation of the planets. They visualized the protoplanetary disk from data computed by Aaron Boley, Sagan Fellow at the University of Florida, using AVL's data visualization plug-in for Maya. The disk was embedded in a turbulent molecular cloud, simulated by Alexei Kritsuk and Michael Norman from the Center for Astrophysics and Space Sciences, University of California-San Diego. Their adaptive mesh refinement simulation was rendered using AVL's custom Amore volume renderer.

AVL staff involved in the project were Donna Cox, Robert Patterson, Stuart Levy, Alex Betts, Matthew Hall, and AJ Christensen.

Narrated by two-time Academy Award winner Jodie Foster, "Life" begins in a grove of towering redwoods, majestic emblems of Northern California. From there, the audience "shrinks" dramatically as it enters a single redwood leaf and then a redwood cell, learning that redwoods are composed of the same basic molecules as all other organisms on Earth. Then the audience witnesses key events since the Big Bang, including the sequence created by AVL. The 25-minute show ends with a review of geological evidence of the connectedness of all living things on Earth. It will play at Morrison Planetarium through late 2011.

GRANT EXPANDS TEXT-MINING RESEARCH

John Unsworth, dean of the Graduate School of Library and Information Science at the University of Illinois, English department faculty member Ted Underwood, and a team of fellow researchers will explore text-mining as a tool for understanding the humanities through a two-year grant awarded to Stanford University. Unsworth will serve as co-principal investigator along with Michael Welge, director of the Automated Learning Group at NCSA; Stanford University librarian Mike Keller will serve as a principal investigator, while Matthew Jockers assists as project director.

The grant of $761,000 from The Andrew W. Mellon Foundation will fund use cases by Underwood and participants at three other universities: Dan Cohen, from the Center for History and New Media at George Mason University; Tanya Clement, associate director of digital cultures and creativity at the University of Maryland; and Franco Moretti, the Danily C. and Laura Louise Bell Professor of English and Comparative Literature at Stanford.

The grant comes at a time of increasing interest in text mining as a technique for producing new research insights into the humanities. It will expand on work completed as part of three other Mellon-supported projects:

- **The Software Environment for the Advancement of Scholarly Research (SEASR)**, which focuses on the development of leading-edge digital humanities initiatives;
- **The NORA project**, a two-year project to produce software for discovering, visualizing, and exploring significant patterns across large collections of full-text humanities resources in existing digital libraries;
- **Metadata Offer New Knowledge (MONK)**, a continuation of the NORA project with co-PI Martin Mueller, at Northwestern University, now available as a library service to faculty, staff, and students at all Committee for Institutional Cooperation institutions (which includes all Big 10 universities and the University of Chicago).

Goals of the project include sharing research findings through peer-reviewed publications in print and online, as well as the further development of infrastructure for text mining. Software development will focus on creating or adapting SEASR modules to explore specific research questions from the use cases and on extending work done in MONK to allow researchers to assemble their own collections from digital repositories. The main emphasis will be on developing, coordinating, and investigating research questions posed by the participating humanities scholars.

JONGENEEL DRIVES BIOMEDICAL PROGRAM

Victor Jongeneel joined the University of Illinois at Urbana-Champaign as a senior research scientist at both the Institute for Genomic Biology (IGB) and NCSA. He is developing a biomedical informatics program that brings together resources and expertise at both research centers and across the Illinois campus.

Jongeneel most recently was the vice president of research and a professor of computational biology at the Cyprus Institute, as well as an associate professor at the Center for Integrative Genomics, University of Lausanne, and a member of the Ludwig Institute for Cancer Research. Previously, he was founding director of the Swiss Bioinformatics Institute and later led its Vital-IT High-Performance Computing Center. He received a PhD in microbiology and immunology from the University of North Carolina at Chapel Hill and a Lic.Sc. in natural sciences from the University of Lausanne.

DOE INCITE AWARDS INCLUDE BLUE WATERS STAFF, COLLABORATORS

The U.S. Department of Energy projects that will receive 1.7 billion processor hours of supercomputing time through its Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program include many researchers with ties to NCSA. They include:

NCSA staffer Brett Bode, software development manager for the Blue Waters sustained-petaflop supercomputer project, is a co-principal investigator for the project Prediction of Bulk Properties Using High Accuracy *ab initio* Methods Interfaced with Dynamical Calculation, which has been renewed after receiving an INCITE grant in 2010. His fellow investigators are Iowa State researchers Theresa Windus, Mark Gordon, Monica Lamm, and Michael Schmidt, and Graham Fletcher from Argonne National Laboratory. Lamm, Windus, and Gordon also have a Petascale Computing Resource Allocation (PRAC) from the National Science Foundation, which enables them to work with NCSA staff to prepare their chemistry codes for Blue Waters.

Illinois computer science professor William Gropp (who is also the deputy director for research of the Institute for Advanced Computing Applications and Technologies and a co-principal investigator for the Blue Waters project) is a co-principal investigator for two projects that have been renewed: Performance Evaluation and Analysis Consortium End Station and Scalable System Software for Performance and Productivity.

Klaus Schulten, leader of Illinois' Theoretical and Computational Biophysics Group, is the principal investigator for a renewed project on Sculpting Biological Membranes by Proteins. Schulten has also been awarded a PRAC to prepare the NAMD molecular dynamics code for Blue Waters.

Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 4Hz will be carried out by Thomas H. Jordan, University of Southern California; Jacobo Bielak, Carnegie Mellon University; Po Chen, University of Wyoming; Yifeng Cui, University of California-San Diego; Philip J. Maechling, University of Southern California; and Kim Olsen, San Diego State University. Jordan and Bielak are also the lead investigators for a Blue Waters PRAC.

Robert Sugar, University of California-Santa Barbara, will use DOE supercomputers for Lattice QCD simulations, with a team of other investigators. Sugar is also the lead investigator for a Blue Waters PRAC.

Michael Norman, University of California-San Diego, is one of the investigators for a project investigating How High Redshift Galaxies Reionized the Universe. He is also the co-PI for a Blue Waters PRAC project.

In addition, Michael Klein and Axel Kohlmeyer, Temple University, are two of the investigators on the project Coarse Grained Molecular Dynamics Studies of Vesicle Formation and Fusion. Both also are involved with NCSA through the CyberChem collaborative, which examines the application of new computing technologies to the chemical sciences.

To learn more about all of the 2011 INCITE awardees, visit: **www.science.energy.gov/ascr/INCITE/**.

NCSA, MAYO EXPLORE GENETIC VISUALIZATION TECHNIQUES

Biomedical researchers are generating a tremendous amount of genomic data about cancer, which has the potential to improve clinicians' ability to diagnose, treat and prevent the disease.

But in order for this complex, heterogeneous data to be useful in a clinical setting, it must be clear and easy to understand, with the relevant information drawn from the overwhelming flood. Researchers at NCSA, Mayo Clinic, and the Genomic Institute of Singapore have begun a pilot project to develop an effective way to visually present genomic data to clinicians. The project is one of several being carried out by the Mayo Illinois Alliance for Technology-Based Healthcare, a joint effort launched in 2010.

The goal is to "bridge the gap between research and clinicians," says Michael Welge, who leads the data-intensive technologies and applications research team at NCSA. Welge and Frank Prendergast of the Mayo Clinic are co-principal investigators. "How do you visually represent information from the research laboratory to the clinician so the clinician can use this in their workflow?"

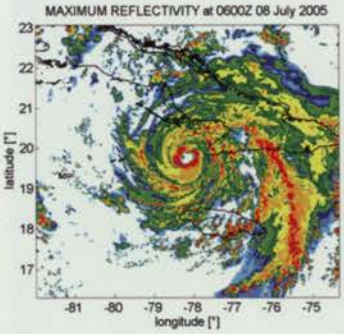
Welge's team brings substantial data visualization expertise to the project, while the team from Singapore, led by Edison Liu and Pauline Ng, provides insight into the research perspective on the data and how it is currently visually represented. Clinicians from Mayo and other hospitals, including Carle Hospital in Urbana, Illinois, explain their typical workflow and how they could use genomic data in diagnosis and in formulating treatment plans.

The plan is to have an initial prototype or mockup this spring; this will be used as the basis for follow-on proposals and research. Welge cautions that they will not get it right the first time, but he thinks a system could be ready for clinical deployment in two to five years.

While Welge's team frequently tackles data visualization challenges, the potential impact of the cancer genome project is particularly exciting. In fact, former NCSA'er Colleen Bushell, now the head of product development for spin-off company RiverGlass, returned to the center part-time specifically to work on this project.

RAPID INTENSIFICATION OF HURRICANES

Greg McFarquhar, University of Illinois at Urbana-Champaign



Maximum radar reflectivity derived from modeled hydrometeor fields of Hurricane Dennis after its rapid intensification and before landfall. These simulations conducted with the Weather Research and Forecasting model are being used to determine how intense vertical velocities cause and/or respond to rapid intensification of tropical cyclones.

It is well known that transformations between phases of water—vapor, liquid, ice—result in latent heating that ultimately affects tropical cyclone intensity. A quantitative understanding of the distribution of cloud microphysical processes releasing this energy and relating to the development of updrafts and downdrafts, however, has not been developed, which challenges forecasters.

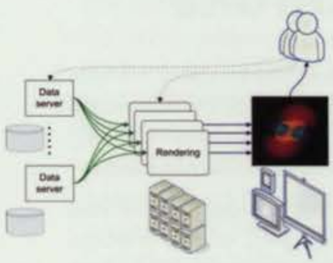
Greg McFarquhar and his colleagues at the University of Illinois at Urbana-Champaign configured the Weather Research and Forecasting model with one kilometer grid spacing and two-minute output frequency to simulate Hurricane Dennis (2005), which was observed during the NASA Tropical Cloud Systems and Processes campaign. NCSA's Abe provided the computational resources for this simulation, which spanned from Dennis' tropical storm through mature hurricane stage and second landfall over Cuba. In particular, 256 processors were used for integration of the model and an additional 16 processors for writing the standard and added latent heat output. It took about 100 hours of real time to complete the 66-hour simulation. NCSA has since proven particularly useful for analyzing the approximately 12 terabytes of data post-processed from this simulation.

To identify potential precursors to the rapid intensification of Dennis, statistical distributions of simulated vertical velocity and latent heat within various horizontal, vertical, and temporal frameworks were constructed. The team found that during the approximately 24-hour period preceding the onset of the most rapid intensification, upper-tropospheric vertical velocity frequency distributions continually broadened while the outliers of these distributions converged toward the simulated tropical cyclone center. Although a clear increase and concentration of latent heating toward the tropical cyclone center occurred, it was only after the onset of and during this most rapid intensification, when lower-to-mid-level vertical velocity frequency distributions broadened and more effectively forced the phase changes of water.

The team presented their work at many conferences, including the 29th Conference on Hurricanes and Tropical Meteorology in 2010.

DISTRIBUTED VISUALIZATION

Andrei Hutanu, Louisiana State University



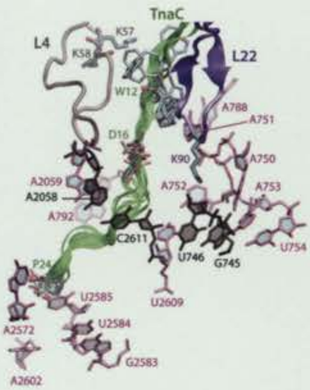
eaviv is a visualization application distributed in three components connected by high-speed networks: data, rendering, and viewer.

Scientific research is increasingly dependent on simulation and analysis requiring high-performance computers, distributed large-scale data, and high-speed networks. Andrei Hutanu of LSU leads a team addressing fundamental issues in distributed visualization design and implementation, where the network services represent a first-class resource. They built a distributed visualization system, eaviv, and a distributed visualization application optimized for large data, high-speed networks and interaction. eaviv connects Spider at LSU's Center for Computation & Technology (CCT), NCSA's Lincoln and accelerator clusters, and a cluster at the Laboratory of Advanced Networking Technologies (SITOLA) at Masaryk University in the Czech Republic. The Internet2 interoperable On-demand Network (ION) provides wide-area connectivity to support dynamic network circuit services, and NCSA's mass storage system provided permanent data storage. Applications request and reserve point-to-point circuits between sites as needed using automated control software. eaviv supports distributed collaboration, letting multiple users in physically distributed locations interact with the same visualization to communicate their ideas and explore the datasets cooperatively. The team implemented a ray-casting parallel volume renderer called Pcaster as the rendering component to demonstrate the distributed pipeline's workflow. Compared to parallel volume renderers in existing software, Pcaster is a purely GPU-based volume renderer and image compositor supporting high-resolution rendering. Pcaster asynchronously couples with parallel data servers for network-streamed data input. The team tested Pcaster with data sets up to 64 gigabytes per timestep and achieved interactive frame rates of five to 10 frames per second on Lincoln to produce render images of 1,024 x 1,024 resolution. The eaviv system's configurable architecture also allows it to run with a local data server and a single renderer, making it a desktop tool for small-scale local data.

This research was published in 2010 in *Scalable Computing: Practice and Experience and Computing in Science and Engineering*, as well as presented at the TeraGrid 10 conference.

MECHANISMS OF PROTEIN SYNTHESIS BY THE RIBOSOME

Klaus Schulten, University of Illinois at Urbana-Champaign



Selected residues of the 23S rRNA, the portions of ribosomal proteins L4 and L22 forming the exit tunnel's constriction site, and ten models of the nascent chain found to be consistent with cryo-EM data. 23S rRNA residues displayed in black represent bacterial sequence signatures.

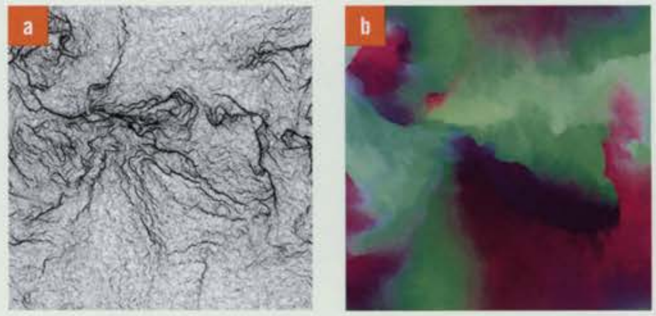
Modeling organisms across many levels of organization, from molecules to cells to networks, while utilizing the advances in physical theory and computing, keeps Klaus Schulten and his group at the University of Illinois at Urbana-Champaign extremely busy. The fundamental research this team conducts is driven by problems in biomedicine.

The team has developed the molecular dynamics flexible fitting (MDFF) method to combine structural information from X-ray crystallography and cryo-electron microscopy (cryo-EM). Using NCSA's Abe and Lincoln clusters, MDFF was applied to obtain atomic models of the ribosome in different functional states imaged by cryo EM. A recent application of MDFF led to the interpretation of a cryo-EM image of the ribosome bound to the regulatory nascent chain TnaC, revealing how this nascent chain induces stalling of protein synthesis. This work also suggests potential signal relay pathways from TnaC to the peptidyl transferase center (PTC) of the ribosome. Further molecular dynamics simulations employing the MDFF-derived models elucidated how TnaC is specifically recognized by the ribosome. The team has also extended their work on ribosome-channel complexes, having solved the structures of an inactive ribosome-SecY complex, an active ribosome-Sec61 complex, and a ribosome-SecY-nascent-protein complex via MDFF. Simulation of the last complex revealed the spontaneous formation of interactions between the ribosome and the lipid bilayer; these interactions provide insight into the nascent-protein insertion process, which forms the basis of the team's future investigations.

This work, which is funded by the National Science Foundation, the National Institutes of Health, and the Howard Hughes Medical Institute, has been published in the *Proceedings of the National Academy of Sciences*, *Structure*, *Science*, and *Methods*.

MATERIALS MORPHOLOGY EVOLUTION

James P. Sethna, Cornell University



Theoretical dislocation fractal morphologies of cellular structures from simulations. The image on the left (a) shows the net dislocation density and on the right (b) is a color representation of the local lattice rotation. When the simulations are compared with experimental work conducted by others, a striking morphological similarity between theory and experiment is noted.

James P. Sethna and his team at Cornell University study dislocation dynamics in materials. One of their computational endeavors explores the dynamic evolution of materials under stress, looking at plasticity and failure of crystalline materials.

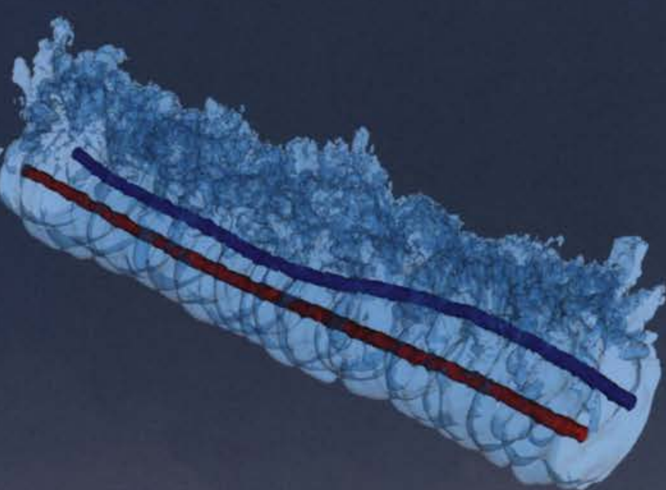
When a single crystal is bent, it can yield through the motion of dislocations, line defects in the crystalline lattice that form complex cellular structures. These mesoscale structures are too large for simulations of atoms or even individual dislocations and pose a serious challenge to "atoms to airplanes" multiscale modeling. Simulations on NCSA's Lincoln and Abe clusters let the team explore their theory of dislocation dynamics in two- and three-dimensional simulations of polycrystals and deformed metals. They also were able to fine-tune their code, which works both in serial and parallel mode, and modify the algorithms to work with GPUs. The simulations showed non-fractal grain boundary formation at high temperatures and fractal cell structure formation at low temperatures. They also exhibit a realistic plastic evolution; cells shrink and domains rotate in a self-similar fashion as external strain is applied.

Their work, which is funded by the Department of Energy's Office of Basic Energy Sciences, was published in *Physical Review Letters* in 2010.

CONTRAIL CL

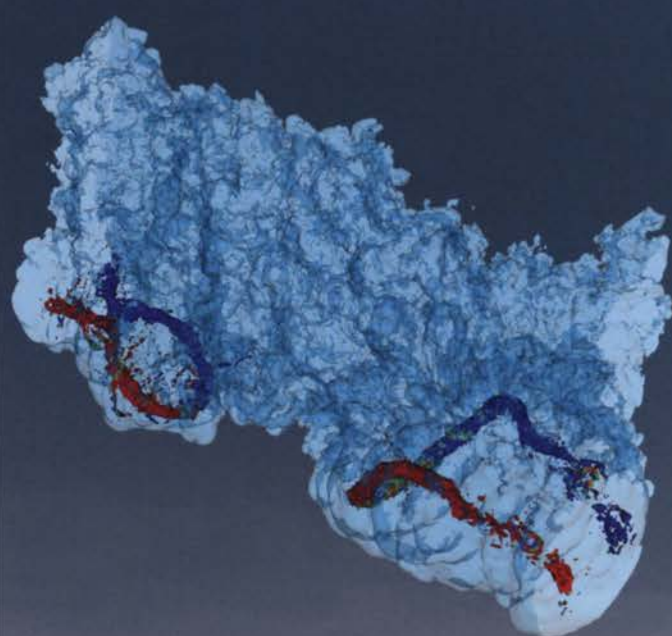
1

Contrails form in aircraft wakes, where the aerodynamics of flight that produce lift also create pairs of strong, counter-rotating vortices. This series of images shows the evolution of the vortex cores (opaque red and blue surfaces) and how they affect the distribution of jet exhaust material (transparent green/blue surface) that forms the contrail. At 65 simulation seconds, the vortices are well defined and parallel to the flight direction.



2

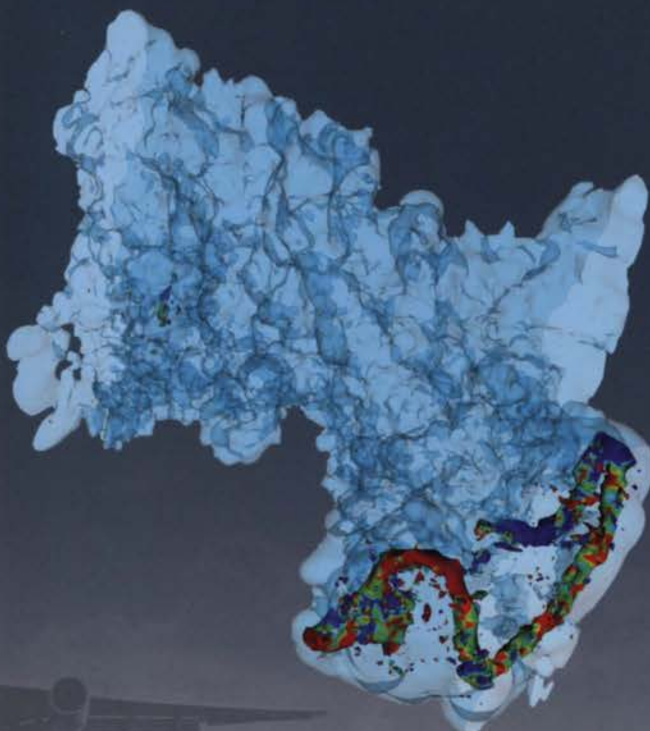
An instability causes small perturbations of the parallel vortices to grow, and the vortices eventually link to form vortex loops. At 120 simulation seconds, a loop has formed and is beginning to expand in the spanwise direction.



LOUDS

3

At 210 simulation seconds, the loop has become very distorted due to mutual induction of different portions of the vortices. The chaotic interaction of the vortices then leads to quick dissipation of the organized system. Even after the vortices are gone, their effect can be seen in the periodic, puffy pattern characteristic of thick contrails.



THE CLIMATE RESEARCH COMMUNITY SUSPECTS THAT aviation impacts global climate by changing cloud cover, but the extent of this effect is very uncertain. That's the focus of a Stanford University project led by Mark Jacobson and Sanjiva Lele. Their team, including PhD candidate Alexander Naiman, is studying the impact of commercial aviation on climate.

The direct effect of aircraft on clouds can be seen by looking up on the right day: Under certain atmospheric conditions, airplanes produce condensation trails, or contrails, which are manmade ice clouds. There is also an indirect effect, in that the exhaust products from jets can induce cirrus cloud formation where clouds might not have formed otherwise. Increasing cloud cover in these ways affects climate by changing the radiative balance, but the change must be carefully studied to determine whether it warms or cools. Clouds can have either a cooling or warming effect depending on their specific properties, and this is where the uncertainty lies.

To understand the cloud properties better, Naiman is conducting research using NCSA's Abe, running a Large Eddy Simulation (LES) using a highly scalable parallelized code developed at Stanford. The LES models the formation and development of contrails, simulating both fluid dynamics and ice microphysics. The simulations start with the wake of a commercial airliner at a cruise condition and continue for 20 minutes of simulation time. The end result is a data set that provides 3D fields of ice size and spatial distribution that allows the calculation of radiative properties of the contrail.

To date, simulations have varied conditions such as aircraft type, ambient humidity, and wind shear. Future work is planned to extend simulation times out to several hours, investigating the transition from linear contrails to diffuse cirrus clouds.

In addition to calculating the properties of individual contrails under a range of conditions, this work has also led to the development of a parameterized model of contrail dynamics. The simple parameterization is used as a subgrid scale model within a large-scale atmospheric simulation, predicting the evolution of individual contrails based on parameters provided by the large-scale simulation. The large-scale simulation is being used to improve estimates of the overall effect of aviation on climate.

Project results have been published in *Atmospheric Chemistry and Physics* in 2010, the *Journal of Computational Physics* in 2011, and also presented in 2009, 2010, and 2011 at meetings of the American Institute of Aeronautics and Astronautics, the American Physical Society Division of Fluid Dynamics, and the American Geophysical Union.

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